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Micropipes and surface energy of compound semiconductors

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In the compound semiconductors, large micropipes are produced in the grown single crystals or the epitaxially grown thin films. The origin of these micropipes have been proposed by Frank's prediction, where the equilibrium radius (r) of the hollow core is determined by the force (F) balance between surface energy (γ) and the strained energy around dislocation core,

$$dF = 2\pi\gamma dr - \frac{\mu b^2}{8\pi^2 r^2} 2\pi r dr .$$

If Burger's vector (b) exceeds the order of magnitude 10 Å, such a dislocation is only in equilibrium with an empty tube at its core.
Using physical properties of SiC, the radius of micropipe is predicted to be less than 10 Å, which is too small than expected from the experimental observations. Furthermore, the solvent process for SiC crystal growth, the generation of micropipes is highly depressed. For the liquid-solid interface applying the 1/10 of the vacuum-solid surface energy, the predicted radius becomes 10 times larger than that of vacuum-solid interface. This disagreement between the experimental result and the prediction suggests the another origin of the micropipe occurrence.
One possibility is the environmental dependency of the chemical potentials. In this study, ab-initio calculations of surface energy of 4H-SiC have been performed using VASP(Vienna Ab-initio Simulation Package). For the polar surface of (0001) shows 7.6J/m^2 for C-rich side, and 2.8J/m^2 for Si-rich side. The perpendicular surfaces against the polar surface show 3.5-4.5J/m^2. This calculated results consistently explain the experimental results of the flat (0001) surface and the closeness of the micropipes of the grown crystals during the solvent processes.

References:

[1] F. C. Frank, Acta Cryst., **4** (1951), 497-501.

Table 1 Micropipe radius predicted by Frank's equation.

	Rigidity modulus μ [10^{11} erg/cm^3]	Surface energy γ [erg/cm^3]	μ/γ [cm^{-8}]	dislocation radius for b=10Å [Å]
Cu	4.4	1400	0.32	4
NaCl	1.5	155	0.10	12
SiC	25.0	5000 (vacuum)	0.20	6
SiC	25.0	500 (liquid)	0.02	63